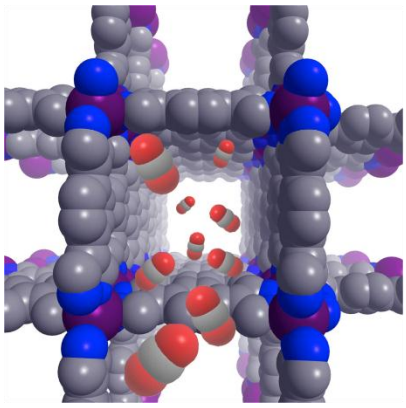
Center for Gas Separations Relevant to Clean Energy Technologies (CGS)
EFRC Director: Berend Smit
Lead Institution: University of California, Berkeley

Mission Statement*: To develop new strategies and materials that allow for energy efficient gas separations based on molecule-specific chemical interactions, with a focus on carbon capture.*

The separation of mixtures of volatile molecules presents a critical issue in the clean use of existing fuels and in the generation of alternative fuels. In particular separation of CO_2 is at present one of the major barriers for large scale CO_2 sequestration. For example, the conventional technology for capturing CO_2 from the effluent stream of a power plant may require as much as 25% of the electricity being produced.



The EFRC will focus on developing new strategies and materials for selective gas capture and separation based on molecule-specific chemical interactions.

The scientific challenge is to remove the fundamental scientific barriers that currently prohibit the efficient gas separations essential to the development of clean energy technologies. In gas separations these challenges are significant. The differences between the relevant gas molecules are small and therefore we need to use the type of molecular control that is offered by nanoscience to tailor materials that have exactly the right adsorption and diffusion selectivity to enable an economic separations process.

The center brings together personnel with expertise in the following areas of emphasis:

- *Materials Synthesis*: The synthesis of new gas-permeable materials with control over the molecular functionalities to preferentially adsorb gas molecules is essential. Our focus here will be on: (i) generating metal-organic frameworks exhibiting high internal surface areas (up to 4,800 m^2/g) and surfaces lined with robust and tailorable chemical groups and (ii) self-assembled polymer films with synthetic or biomimetic functional units.
- *Materials Characterization*: Detailed atomic-level structural characterization of the new materials will be necessary both before and after exposure to gas samples in order to probe hypotheses on interaction mechanisms. In addition, accurate means of assessing the selectivity, kinetics, and thermodynamics of gas adsorbate binding will be needed to demonstrate efficacy and test computational models.
- *Computational Separations*: A strong computational component to the research will be essential for understanding the chemical interactions at a molecular level, as well as for guiding the synthetic efforts toward materials exhibiting high specificity and tunable interaction energies.

We aim to develop fundamental new means of synthesizing materials with tailored molecular interactions, while generating new options for energy-related gas separations, including separation of CO_2 from power plant flue streams and separation of CO_2 from natural gas deposits.

Center for Gas Separations Relevant to Clean Energy Technologies	
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